

Anhydromethylenecitric acid
144-16-1 | DTXSID60162592

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.45e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.15e-01

Confidence level: 6.48e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Anhydromethylenecitric acid</div> <div>Measured: 2.45e-01</div> <div>Predicted: 2.45e-01</div>	<div>Image not found</div> <div>Butanoic acid, 4,4'-dioxybis[4-oxo-</div> <div>Measured: 1.42e-01</div> <div>Predicted: 1.42e-01</div>	<div>Image not found</div> <div>Chelidonic acid</div> <div>Measured: 7.77e-02</div> <div>Predicted: 1.22e-01</div>
<div>Image not found</div> <div>D-Glucose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>	<div>Image not found</div> <div>Galactose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>	<div>Image not found</div> <div>alpha-d-glucopyranose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>
<div>Image not found</div> <div>D-Mannose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>		

